

Theoretical Study of Thermodynamic and Elastic Properties of $Ti_{50}Be_{34}Zr_{16}$ BMG – A Pseudopotential Method

Alkesh L. Gandhi¹, Aditya M. Vora²

¹Assistant Professor, ²Associate Professor

¹Department of Physics, B. V. Shah (Vadi-Vihar) Science College, C. U. Shah University, Wadhwan, Gujarat, India

²Department of Physics, University School of Sciences, Gujarat University, Ahmedabad, Gujarat, India

ABSTRACT

Pseudo-Alloy atom model under pseudopotential concept is effectively exploited to determine the elastic and thermodynamic properties of a bulk metallic glass (BMG). Such a study helps in finding novel applications of BMG. Here, the vibrational or phonon dynamics of $Ti_{50}Be_{34}Zr_{16}$ BMG has been theoretically studied in terms of longitudinal and transverse mode of phonon eigen frequencies. The electron-ion interactions are represented by a well-established model potential with widely accepted local field correction functions. The computed results of the phonon dispersion curves (PDC) produce respective phononic nature in the amorphous glassy alloy.

Keywords: Bulk metallic glass, Model potential, Phonon dispersion curve, Thermodynamic properties, Elastic properties

1. INTRODUCTION

The discovery of bulk metallic glasses (BMGs) has encouraged extensive research interest because of their exciting technological potentials for novel applications and scientific importance in understanding their unique properties like high fracture strength, soft magnetism, excellent corrosion and wear resistances, anomalous electronic transport properties etc. BMGs have become popular as the new engineering materials in several applications extended from the common window glass to sports materials, prosthetic devices, scientific instruments, fashion jewelries, data storage devices in digital media, cellphone case, outer body of space vehicle etc. A BMG displays liquidus temperature below melting points of its configurational elements and behaves as an atomically frozen liquid, which forms a unique amorphous atomic structure of a glassy solid having high yield strength and high elastic limit under shock impact conditions as it is lacking slips planes [1,2].

$Ti_{50}Be_{34}Zr_{16}$ BMG has high glass-forming ability, good castability, good printability and unique characteristics [3].

The Zr based BMGs are used to prepare complex shaped optical mirrors with smooth surface and good reflectivity with high dimensional accuracy. Ti based BMGs are ideal materials for bio-medical applications because of their low density, higher biocompatibility and good corrosion resistivity.

Here, $Ti_{50}Be_{34}Zr_{16}$ BMG is very first time theoretically investigated in terms of its elastic and thermodynamic properties through vibrational dynamics using pseudopotential theory [1,2]. In order to attain the phonon eigen frequencies, the two main computational approaches used have been developed by Hubbard-Beeby (HB) [4] and Takeno-Goda (TG) [5,6]. The screening influence on the BMG properties has been studied by five local field correction functions viz. Hartree (H) [7], Taylor (T) [8], Ichimaru-Utsumi (IU) [9], Farid *et al.* (F) [10] and Sarkar *et al.* (S) [11].

Since past data is not available in the literatures for this BMG, its pair correlation function is theoretically generated from the interatomic pair potentials. A suitable, well-known and accepted model potential – Shaw's constant core model potential [12] is successfully exploited here for this investigation. Some of the important elastic and thermodynamic properties viz. Young's modulus (Y), modulus of rigidity (G), Isothermal bulk modulus (B_T), Poisson's ratio (σ), transverse sound velocity (v_T), longitudinal sound velocity (v_L), Debye-temperature (θ_D) are theoretically computed from PDCs of this BMG [1,2].

2. THEORETICAL METHODOLOGY

A well-established Pseudo-Alloy Atom (PAA) model [1, 2] is adopted for investigating vibrational properties of $Ti_{50}Be_{34}Zr_{16}$ BMG elucidation on Shaw's constant core model potential [12] is,

$$W(q) = - \frac{8\pi Z}{\Omega_0 q^2} \left[\frac{\sin q r_c}{q r_c} \right] \quad (01)$$

here, Z is valence, q is the wave vectors and Ω_0 is atomic volume. The model potential parameter r_c can be obtained by fitting either to some experimental data or to realistic form-factors or other data relevant to the properties investigated.

The pseudopotential parameter is so fixed that it may generate a pair correlation functions accurately consistent with the experimental data found in the literature. Instead of Vegard's law, the electron-ion interactions are explained by PAA model [1,2]. The ternary BMG system $A_p B_q C_r$, where p, q, and r are the proportionate concentration of the concerned element, is like a multi-component fluid containing bare ions and mixed ions immersed in a uniform electron gas. If the pair potentials of the single components

are known, the mean effective density dependent interatomic pair potential $V(r)$ can be derived successfully [13]. Here, the fundamental component pair potential [7, 12, 14] is given by,

$$V(r) = V_s(r) + V_b(r) + V_r(r). \quad (02)$$

The contribution from the s-electron to the pair potential $V_s(r)$ is then,

$$V_s(r) = \left[\frac{Z_s^2 e^2}{r} \right] + \left(\frac{N_s}{\pi^2} \right) \int F(q) \left[\frac{\sin(qr)}{qr} \right] q^2 dq \quad (03)$$

Where, r is the core radius. The number of s-valance electron $Z_s \cong 1.5$ is obtained by integrating the partial S-density of states, which result from the self-consistent band structure computation for the entire 3d series and 4d series. The number of d-electrons contributing to the pair-potential is Z_d . The d-state radii r_d and the nearest neighbor coordinate number N are given by [1, 2, 15],

$$V_b(r) = -Z_d \left(1 - \frac{Z_d}{10} \right) \left(\frac{12}{N} \right)^{\frac{1}{2}} \left(\frac{28.6}{\pi} \right) \left(2 \frac{r_d^3}{r^3} \right) \quad (04)$$

Table 1: Input parameters and Constants useful in the computational work.

Z	Z _s	Z _d	R _d (au)	R _s (au)	Ω ₀ (au) ³	N _c	M (amu)	r _c (au)
3.32	1.50	1.65	1.45	1.9465	102.56	7.92	67.54	0.6654

The parameters Z_s, Z_d, r_d and N are determined from band structure data of pure metallic component which are already found in the literature [1, 2, 15] and obtained by the following expressions.

$$Z_d = pZ_{dA} + qZ_{dB} + rZ_{dC} \quad (07)$$

$$Z_s = pZ_{sA} + qZ_{sB} + rZ_{sC} \quad (08)$$

$$r_d = pr_{dA} + qr_{dB} + rr_{dC} \quad (09)$$

$$N = pN_A + qN_B + rN_C \quad (10)$$

Z_A, Z_B, Z_C, Z_D and Z is valency. The PCF $g(r)$ is as important as the interatomic pair potential $V(r)$ in studying a BMG [1, 2, 16].

$$g(r) = \exp \left[\left(\frac{-V(r)}{k_B T} \right) - 1 \right] \quad (11)$$

Where, T is Room temperature and k_B , the Boltzmann's constant.

The mathematical notations and theoretical discussions are found from the respective papers of HB- and TG- approaches [4 – 6, 14, 17 – 19]. In the long wavelength limit of the phonon frequency spectrum, the longitudinal and transverse frequencies are proportional to the wave vectors.

$$\therefore \omega_L = v_L q \quad \text{and} \quad \omega_T = v_T q. \quad (12)$$

The longitudinal and transverse sound velocities (v_L and v_T respectively) are computed from the long-wavelength limits of the PDCs as given in the literatures [1, 2, 4-6]. Young's modulus Y , Isothermal bulk modulus B_T , Modulus

of rigidity G , Poisson's ratio σ and the Debye temperature θ_D are derived by the formulae [1, 2] given below.

$$V_r(r) = Z_d \left(\frac{450}{\pi^2} \right) \left(\frac{r_d^6}{r^6} \right). \quad (05)$$

Here, $V_r(r)$ arises from repulsion of the d-electron muffin-tin orbitals on different sites due to their non-orthogonality. Wills and Harrison [15] studied the effects of the s-band and d-band.

Where, $f(q)$ is the local field correction function, m_e and e are mass and charge of an electron respectively For BMG, the model potential parameter r_s [1, 2, 15] is given below.

$$r_s = \left[\frac{(0.51) r_s^3}{(Z)^{2/3}} \right] \quad (06)$$

Where, r_s is the Wigner Seitz radius of the BMG. The input parameters of s-electron valance (Z_s), d-electron valance (Z_d), d-band radius (R_d), Wigner-Seitz radius (R_s), Volume (Ω_0), Coordination. No. (N), Mass (M) and Core radius (R_c) are used for computation and tabulated in table: 1.

Where, r_s is the Wigner Seitz radius of the BMG.

$$B_T = \rho \left[v_L^2 - \frac{4}{3} v_T^2 \right] \quad (13)$$

$$G = \rho v_T^2 \quad (14)$$

$$\sigma = \frac{1 - 2 \left(v_T^2 / v_L^2 \right)}{2 - 2 \left(v_T^2 / v_L^2 \right)} \quad (15)$$

$$Y = 2G(\sigma + 1) \quad (16)$$

$$\theta_D = \frac{\hbar \omega_D}{k_B} = \frac{\hbar}{k_B} 2\pi \left[\frac{9\rho}{4\pi} \right]^{1/3} \left[\frac{1}{v_L^3} + \frac{2}{v_T^3} \right]^{-1/3} \quad (17)$$

Here, ω_D is the Debye frequency, ρ is isotropic number density.

3. RESULTS AND DISCUSSION:

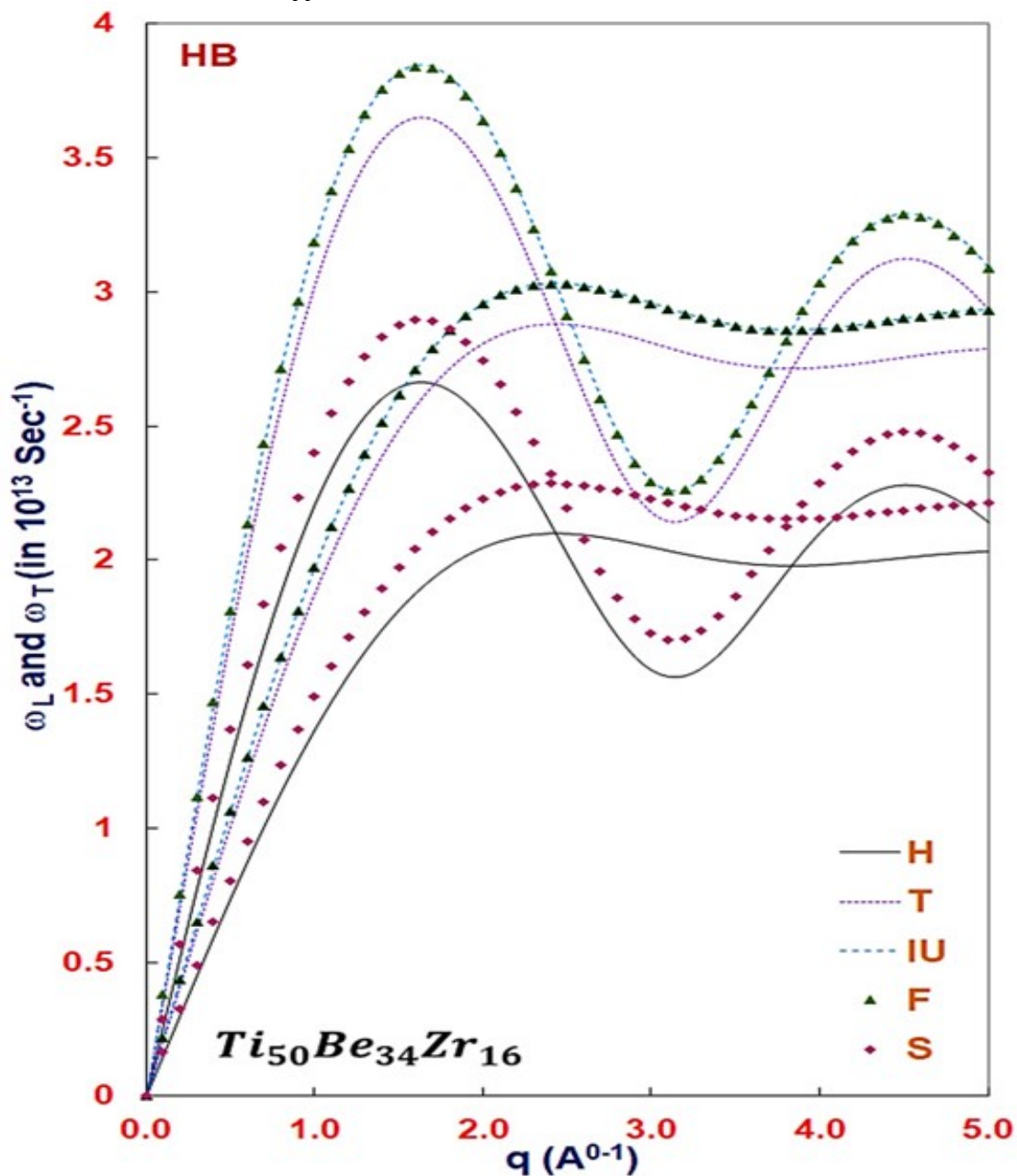
Figures 1 and 2 show the PDCs of for longitudinal and transverse modes of phonon eigen frequencies (ω_L and ω_T sec^{-1}) versus wave vector q (\AA^{-1}) computed with HB- and TG- approaches respectively with the five local field screening functions Viz. H, T, IU, F and S. The obtained phonon dynamical or vibrational properties for this BMG can be compared with the other such and experimentally generated data whenever available.

The inclusion of exchange and correlation effect increases the phonon eigen frequencies for both longitudinal and transverse modes. For the HB-approach, the plot of T-, S- and F- screening functions are lying between those due to H- and IU-screening functions for both branches. In TG-approach, the plots of H-, T- and F- are lying between those of S- and IU-functions for both branches.

The first minimum for the longitudinal frequency (ω_L) in the HB-approach, is found around at $q \approx 3.3 \text{ \AA}^{-1}$ for H- and $q \approx 3.1 \text{ \AA}^{-1}$ for the rest of the functions; in the TG-approach, it is found around $q \approx 2.9, 3.1, 3.1, 3.1$ and

In the HB approach, the first minimum transverse frequencies (ω_T) for all functions are found around $q \approx 3.8 \text{ \AA}^{-1}$; while in TG approach, it is found at $q \approx 4.1, 4.3, 4.3, 4.3$ and 4.9 \AA^{-1} respectively for the H-, T-, IU-, F- and S- functions. For the transverse branch (ω_T), the first maximum is found around at $q \approx 2.3 \text{ \AA}^{-1}$ for F- 2.4 \AA^{-1} for the rest of local field correction functions in HB- approach, In the TG

3.5 \AA^{-1} for H- T-, IU- F- and S- functions respectively. Typically, the dispersion relations express a minimum near q_p , the wave-vector where the static structure factor $S(q)$ of the BMG has its first maximum. The first maximum for the longitudinal frequency ($\omega_{L, \max}$) in the HB-approach is found around at $q \approx 1.6 \text{ \AA}^{-1}$ for all functions; in the TG-approach, it is found around at $q \approx 1.4 \text{ \AA}^{-1}$ for H-function, $q \approx 1.5 \text{ \AA}^{-1}$ for T- IU and F- functions and $q \approx 1.8 \text{ \AA}^{-1}$ for S-function.



approach, it is found around at $q \approx 2.7, 2.8, 2.8, 2.8$ and 3.3 \AA^{-1} for H-, T, IU-, F- and S-functions respectively.

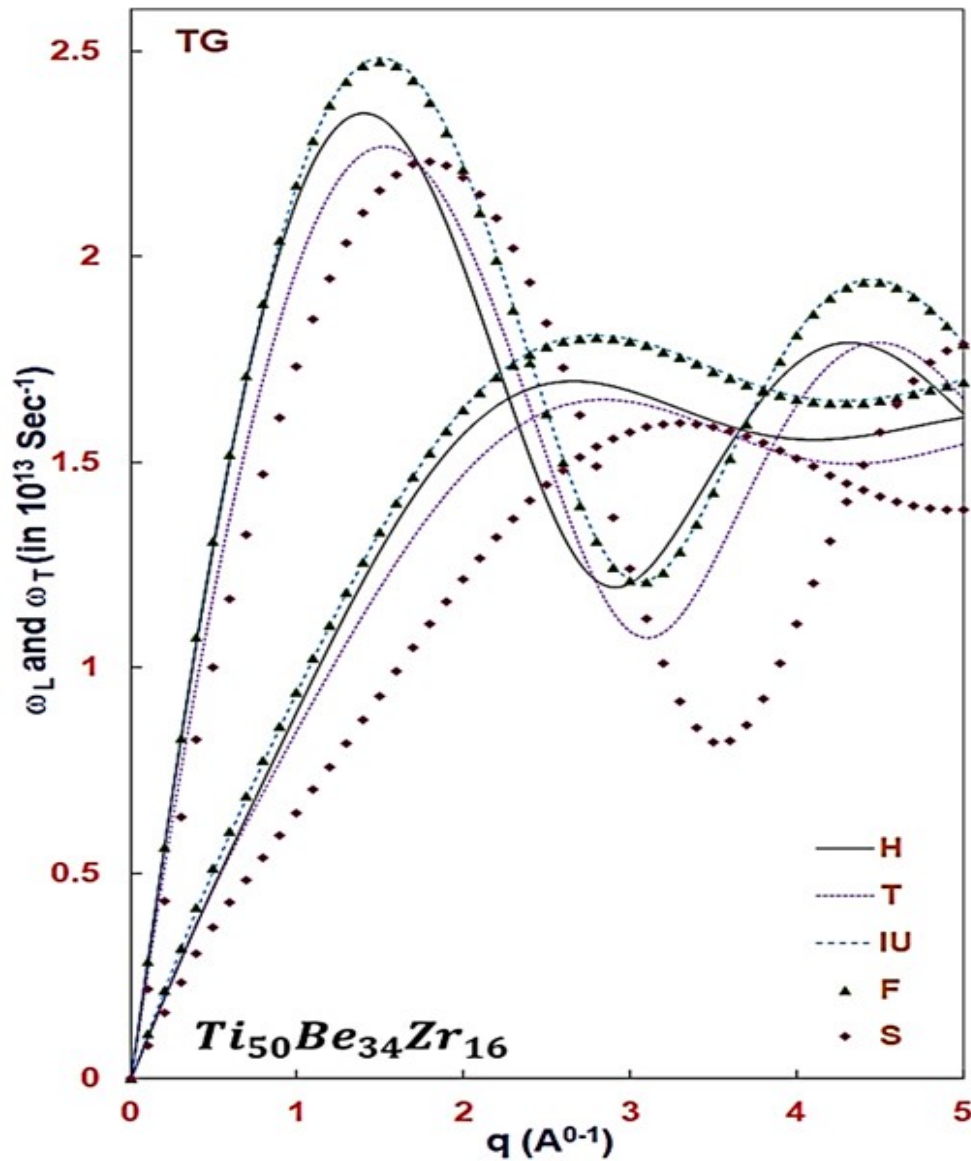


Figure : PDCs of longitudinal and transverse Phonon frequencies for $Ti_{50}Be_{34}Zr_{16}$ BMG using HB approach.

The first crossover position of ω_L and ω_T in the HB-approach is observed at $q \approx 2.4, \text{\AA}^{-1}$ for all local field correction functions. The first crossover position of ω_L and ω_T in the TG-approaches is seen at $q \approx 2.3, 2.4, 2.4, 2.4$ and 2.7\AA^{-1} for H, T-, IU- and F- and S- functions respectively

These both PDCs collectively disclose that the longitudinal mode oscillations are more prominent than that of the transverse one. The instability of the transverse mode oscillations is due to anharmonicity of the atomic vibration in the BMG system. The collective excitations at larger momentum transfer is because of the prominence of longitudinal mode vibrations only.

Table2: Elastic and Thermodynamic properties of $Ti_{50}Be_{34}Zr_{16}$ BMG.

App.	SCR	$v_L \times 10^5$ cm/s	$v_T \times 10^5$ cm/s	$E_T \times 10^{11}$ dyne/s ²	$G \times 10^{11}$ dyne/s ²	σ	$Y \times 10^{11}$ dyne/s ²	θ_D K
HB-approach	H	2.62	1.51	1.69	1.02	0.25	2.54	200.46
	T	3.59	2.07	3.18	1.91	0.25	4.77	274.71
	IU	3.79	2.19	3.54	2.12	0.25	5.30	289.60
	F	3.78	2.18	3.52	2.11	0.25	5.29	289.08
	S	2.85	1.65	2.00	1.20	0.25	3.00	217.96
TG-approach	H	2.67	0.99	2.59	0.43	0.42	1.23	133.76
	T	2.47	1.01	2.10	0.45	0.40	1.27	136.66
	IU	2.69	1.09	2.52	0.52	0.40	1.47	146.89
	F	2.69	1.09	2.51	0.53	0.40	1.48	147.45
	S	2.07	0.82	2.57	0.51	0.41	1.44	126.67

4. CONCLUSION:

It is concluded that the phonon dynamics of $Ti_{50}Be_{34}Zr_{16}$ BMG can be estimated by the PDC generated from HB- and TG- approaches with five local field correction functions, due to H-, T, IU-, F- and S-, with the successful application of the Shaw's model potential, produce all broad characteristics of the dispersion curves and predict for the various useful thermodynamic and elastic properties under investigation. The computed PDCs show extensive features of broad range collective excitations in $Ti_{50}Be_{34}Zr_{16}$ BMG. The dielectric function is significant in the computation of the screening potential due to electron gas and the local field correction functions. The relative effects of exchange and correlation in the selected properties, examined by different local field correction functions, show variations according to the vibrational properties. The thermodynamic properties obtained due to BS-approach are higher than those due to HB or TG-approaches. The complete picture tells the importance of local field correction function as well as the approaches in analysing the properties of the BMG. Since the experimentally or theoretically observed data of most of this BMG are not available in the literature, it is difficult to make any special remarks. However, this investigation proves to be very useful to offer vital information concerning a particular BMG system.

References:

- [1] A. M. Vora, Vibrational Dynamics of Binary Metallic Glasses, Lap Lambert Academic Publishing, Germany (2012).
- [2] A. M. Vora, Vibrational Dynamics of Bulk Metallic Glasses Studied By Pseudopotential Theory, Computational Materials, Ed. Wilhelm U. Oster, Nova Science Publishers, Inc., New York (2009), pp.119-176.
- [3] A. Inou, X.M. Wang and W. Zhang, Rev. Adv. Mater. Sc., Vol. 18, (2008), pp. 1-9.
- [4] J. Hubbard; J. L. Beeby, J. Phys. C: Solid State Phys, (1969), Vol. 2, pp. 556-571.
- [5] S. Takeno; M. Goda, Prog. Thero. Phys., (1971), Vol. 45, pp. 331-352.
- [6] S. Takeno; M. Goda, Prog. Thero. Phys., (1972), Vol. 47, pp. 790-806.
- [7] W. A. Harrison, Elementary Electronic Structure, (1999), World Scientific, Singapore.
- [8] R. Taylor, J. Phys. F: Met. Phys., (1978), Vol. 8, pp. 1699-1702.
- [9] S. Ichimaru; K. Utsumi, Phys. Rev. B., (1981), Vol. 24, pp 7385-7388.
- [10] B. Farid; V. Heine; G. Engel, I. Robertson, J. Phys. Rev. B. (1993), Vol. 48, pp.11602-11621.
- [11] A. Sarkar; D.S. Sen; S. Haldar; D.Roy, Mod. Phys. Lett., B. (1998), Vol. 12, pp. 639-648.
- [12] R.W.Shaw, Phy. Rev., (1968), Vol. 174, p. 769.
- [13] Gupta A.; Bhandari D.; Jain K. C.; Saxena N. S. Phys. Stat. Sol. (b). Vol. 95, (1996), pp. 367-374.
- [14] W. A. Harrison, Pseudopotentials in the Theory of Metals, (1966), W. A. Benjamin, Inc., New York.
- [15] J. M. Wills; W.A. Harrison, Phys. Rev B., (1983), Vol. 28, pp. 4363-4373.
- [16] E. TFaber, Introduction to the Theory of Liquid Metals; (1972), Cambridge Uni. Press: London.
- [17] V. Heine and D. Weaire, Solid State Physics 24, Eds. H. Ehrenreich, F. Seitz and D. Turnbull, Academic Press, New York (1970) p.249.
- [18] L. I. Yastrebov and A. K. Katsnelson, Foundations of One-Electron Theory of Solids, (1987), Mir Publications, Moscow.
- [19] J. M. Ziman, Principal of the theory of the solids, 2nd edition, (1972), Cambridge Uni. Press, London.